Progress in Spray and Combustion Modeling for Internal Combustion Engine Applications: Validation Against ECN Data

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Abstract:

The objective of this presentation is to report on four different projects:

(1) Modeling shock-tubes to engines: A biodiesel-surrogate model consisting of Methyl butanoate and n-heptane was developed and reduced. Several reaction rates were updated based on ab-initio studies. The mechanism predicted combustion characteristics well in 0D, 1D, and 3D spray combustion environment

(2) Combustion modeling for diesel surrogates: A reduced model for n-dodecane (consisting of 103 species and 370 reactions) was developed starting from the Lawrence Livermore detailed mechanism. The reduced mechanism was able to capture the experimental trends available through the ECN and is available for distribution to other ECN modelers world-wide

(3) Large Eddy simulation using a Smagorinsky model: A Smagorinsky based LES turbulence model was implemented in CONVERGE software. The LES model was able to better predict the experimental trends both quantitatively and qualitatively compared to a RANS model

(4) Comparison of diesel with heavy-alcohol-diesel blends: Metabolic engineering efforts at Argonne resulted in the development of Phytol ($C_{20}H_{40}O$). The properties of this alcohol was found to be similar to diesel fuel. Engine experiments reveal that blends of Phytol with diesel fuel produce similar combustion and emission characteristics as diesel fuel

Acknowledgements

Sponsors: U.S. Department of Energy, Office of Vehicle Technology under the management of **Mr. Gurpreet Singh, Mr. Kevin Stork**

Outline

- Modeling: Shock-tubes to Engines

  Collaboration: Chemical Science and Engineering group at Argonne

- Combustion modeling of diesel surrogates:

  Validation with ECN data

  Collaboration: Lawrence Livermore National Laboratory, University of Connecticut

  Data: Sandia National Laboratory

- Large Eddy Simulations using Smagorinsky model

  Collaborations: Convergent Science, Inc.

- Nozzle flow simulations: Comparison of diesel with heavy-alcohol-diesel blends

Modeling: Shock-tubes to Engines

Team members:

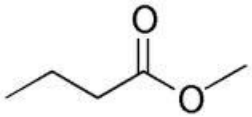
Douglas E. Longman: Argonne

Raghu Sivaramakrishnan, Wei Liu, Mike Davis: Chemical Science and Engineering (Argonne)

Tianfeng Lu: University of Connecticut (UConn)

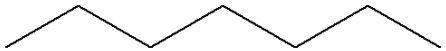
* W. Liu, R. Sivaramakrishnan, M.J. Davis, S. Som, D.E. Longman, T.F. Lu. Development of a reduced biodiesel surrogate model for compression ignition engine modeling. Submitted to the Proceedings of the Combustion institute, 2012

Methyl Butanoate ($C_5H_{10}O_2$)



+

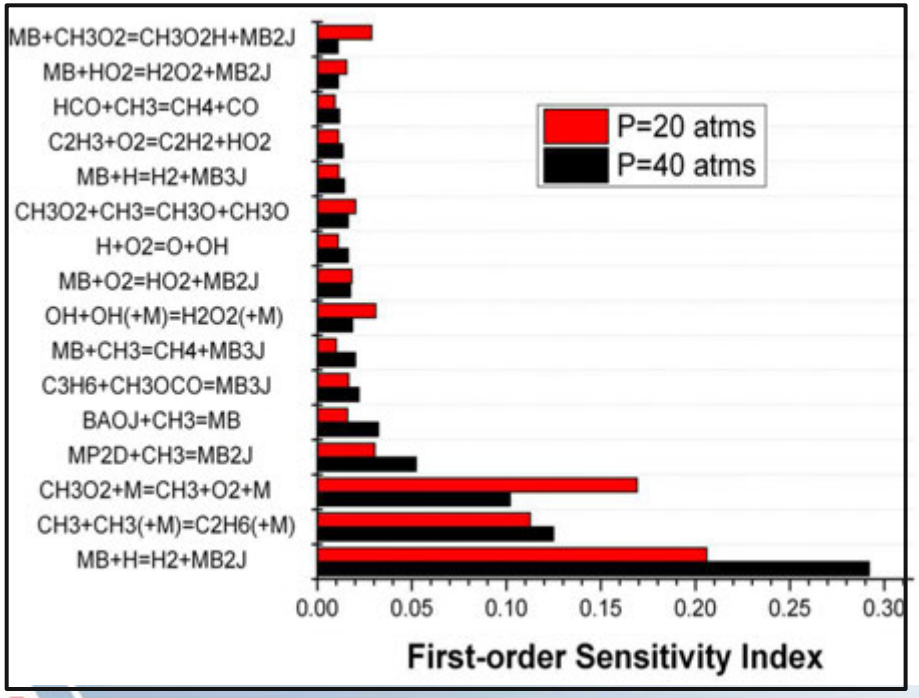
N-heptane(C_7H_{16})



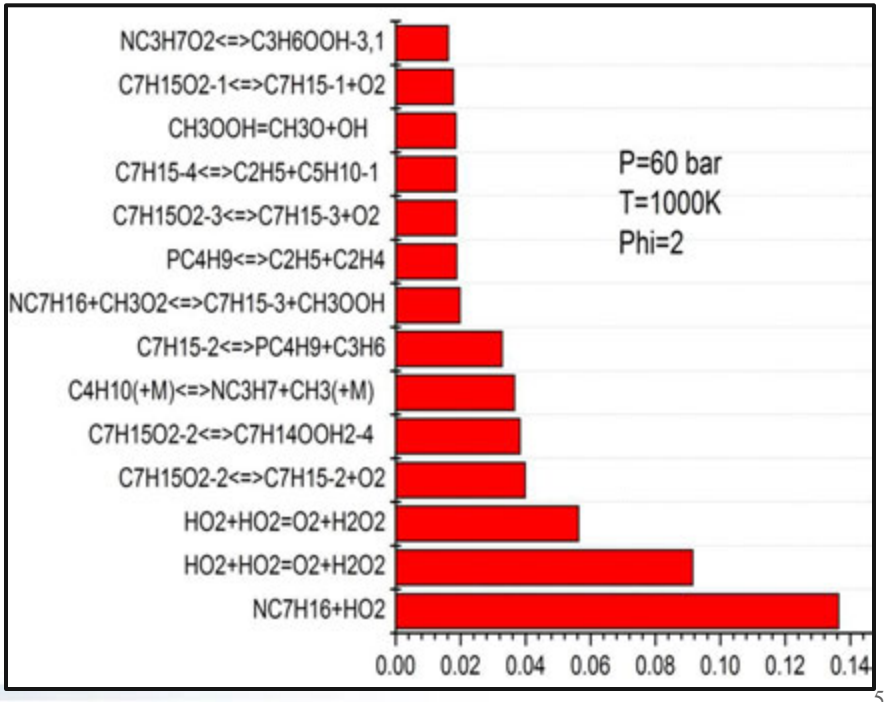
Detailed Mechanism for Biodiesel Surrogate

- A detailed mechanism for Methyl Butanoate (MB) consisting of 262 species and 1529 reactions was assembled in a hierarchical manner.
- This model was then combined with the n-heptane sub-mechanism from Lawrence Livermore National Laboratory. The MB + n-heptane model consists of 661 species and 3019 reactions.
- Swamping effect is observed wherein n-heptane reactions start dominating due to its higher reactivity compared to

Methyl Butanoate



Methyl Butanoate + n-heptane



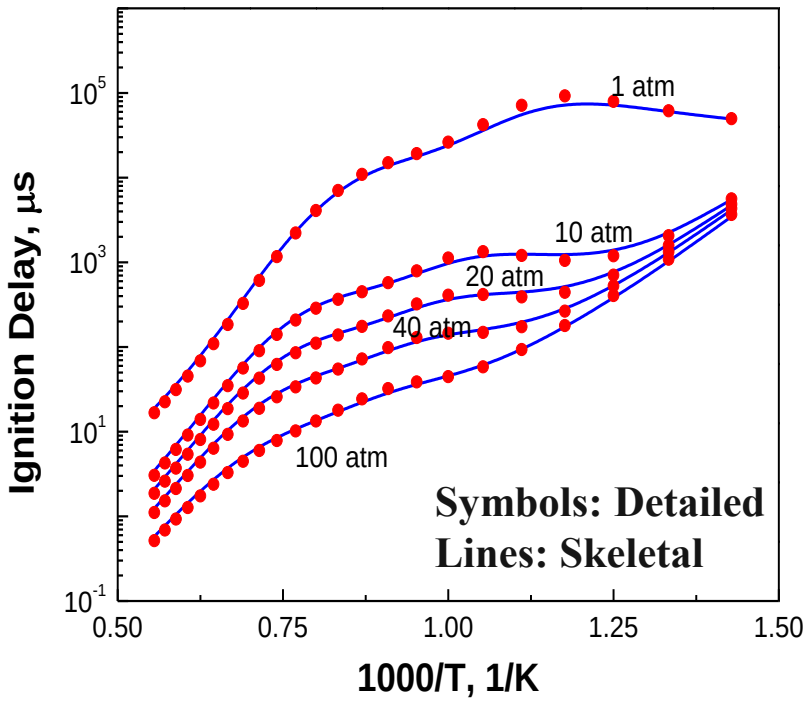
Skeletal Mechanism Development

~ 4.5 times reduction

MB + n-heptane detailed model
661 species, 3019 reactions

DRG – X*, DRGASA, Isomer Lumping

Skeletal Mechanism:
145 species, 869 reactions

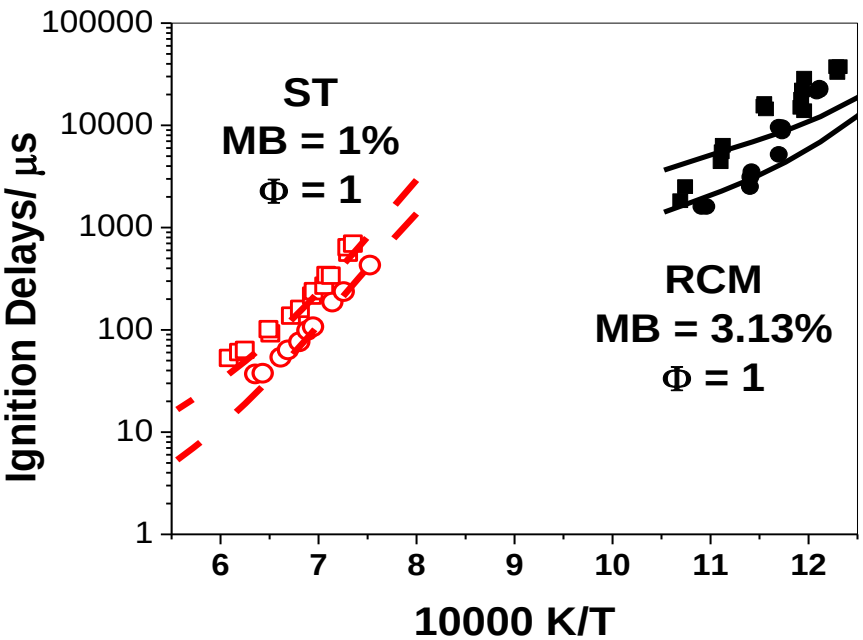


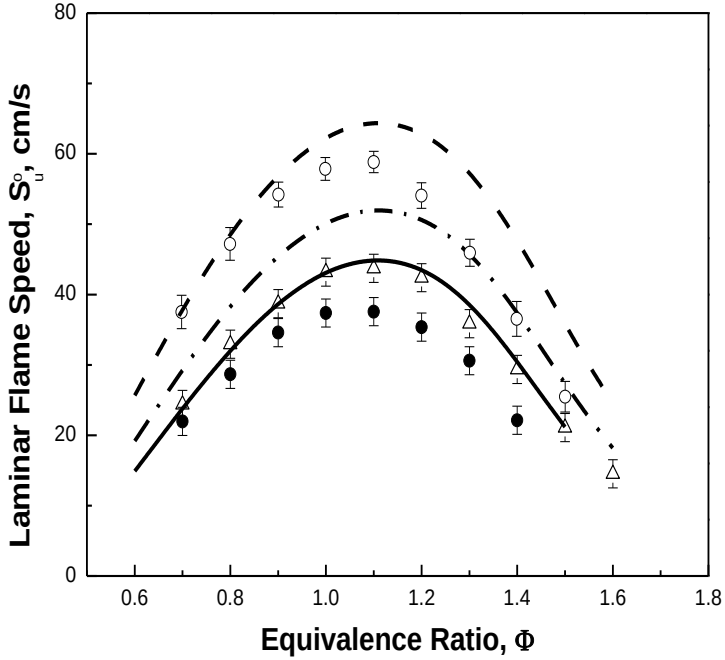
Range of operation:
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

No skeletal mechanism tuning to match any particular data-set!

* **T. Lu, M. Plomer, Z. Luo, S.M. Sarathy, W.J. Pitz, S. Som, D.E. Longman, 1A03.** ***US National Combustion Institute meeting, 2011***

Validation in Idealized Combustion Systems





- In general, the MB model was able to capture the ignition delay data from both shock tubes and rapid compression machine (RCM)
- Laminar flame speeds were also fairly well predicted
- The n-heptane model from LLNL has been validated
- Reliable data for MB + n-heptane mixtures not available

1) Ignition delay data: S. Dooley, H.J. Curran, J.M. Simmie. *Combustion and Flame* (2008)

2) Flame speed data: Y.L. Yang, Q. Feng, F.N. Egolfopoulos, T.T. Tsotsis. *Combustion and Flame* (2011)

3-D Modeling Set-up

Modeling Tool	CONVERGE Source code access for spray and combustion modeling
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 2mm or 4mm Finest grid size: 0.125mm, 0.25mm Gradient based AMR on the velocity and temperature fields Fixed embedding in the near nozzle region to ensure the finest grid sizes
Total grid number	550K-650K for 0.25mm – RANS simulations 1.5-2.0 million for 0.125mm – LES case
Parallelizability	Good scalability up to 48 processors

Turbulence and scalar transport model(s)	RNG k-ε, LES-Smagorinsky
Spray models	Breakup: KH-RT with breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model
Time step	Variable based on spray, evaporation, combustion processes
Turbulence-chemistry interactions model	Direct Integration of detailed chemistry well-mixed (no sub-grid model)
Time discretization scheme	PISO (Pressure Implicit with Splitting of Operators)

Biodiesel: Case set-up

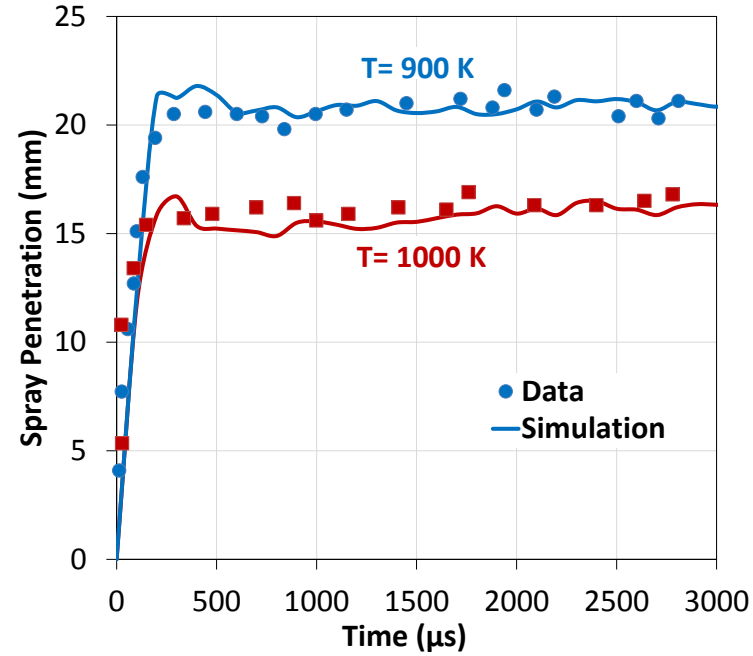
Injection & Ambient conditions for Biodiesel studies at Sandia*

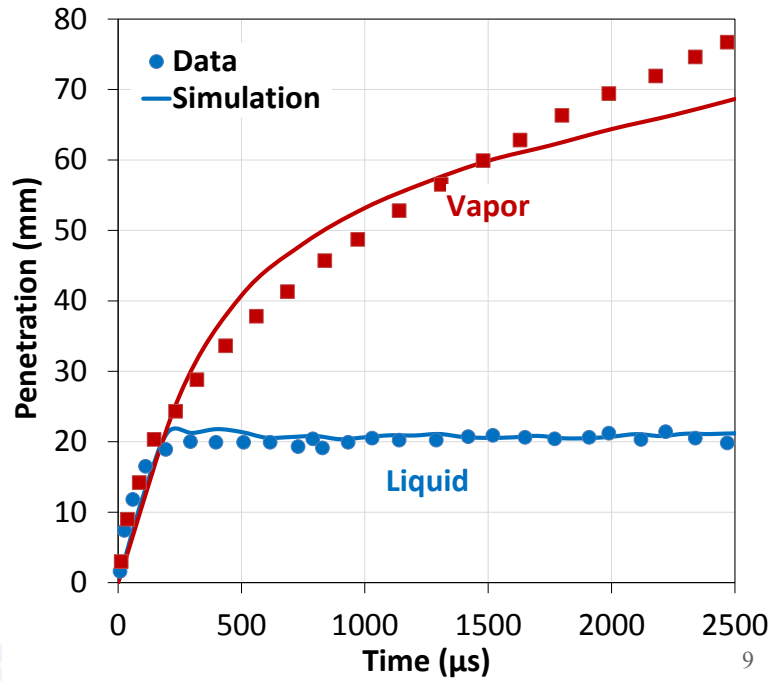
Parameter	Quantity
Injection System	Bosch Common Rail
Nozzle Description	Single-hole, mini-sac
Duration of Injection [ms]	7.5
Orifice Diameter [µm]	90
Injection Pressure [Bar]	1400
Fill Gas Composition (mole-fraction)	N_2=0.7515, O_2=0.15, CO_2=0.0622, H_2O=0.0363
Chamber Density [kg/m³]	22.8
Chamber Temperature [K]	900, 1000
Fuel Density [kg/m³]	877
Fuel Injection Temperature [K]	363

*Pickett & Co-workers (2011) *Personal Communication*
JG Nerva, CL Genzale, JMG Oliver, LM Pickett. Fundamental Spray and Combustion Measurements of Biodiesel under Diesel steady conditions. *Under preparation*

Non-reacting spray characteristics well predicted by the simulations!

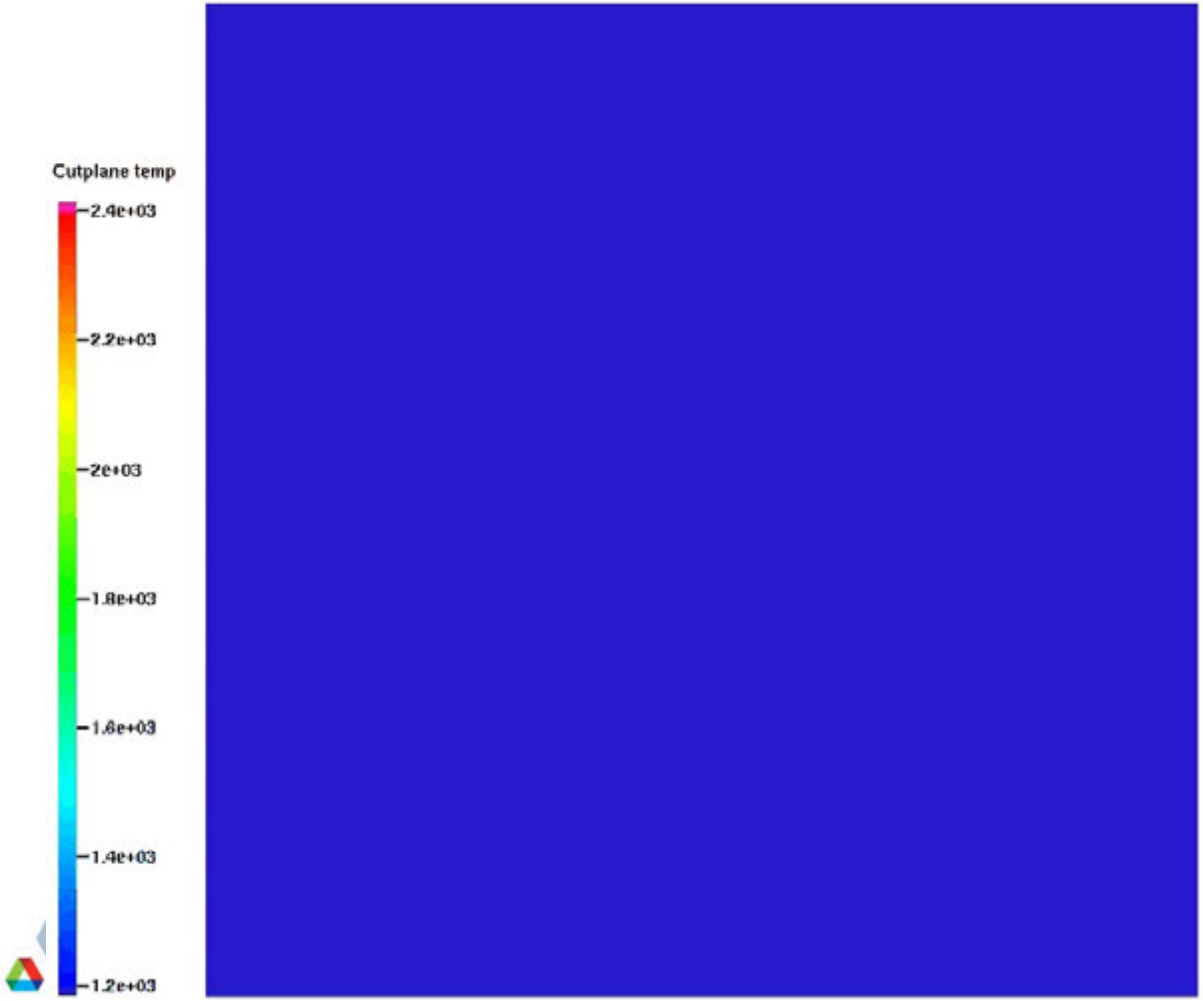
Som et al. ASME ICE2011-60051





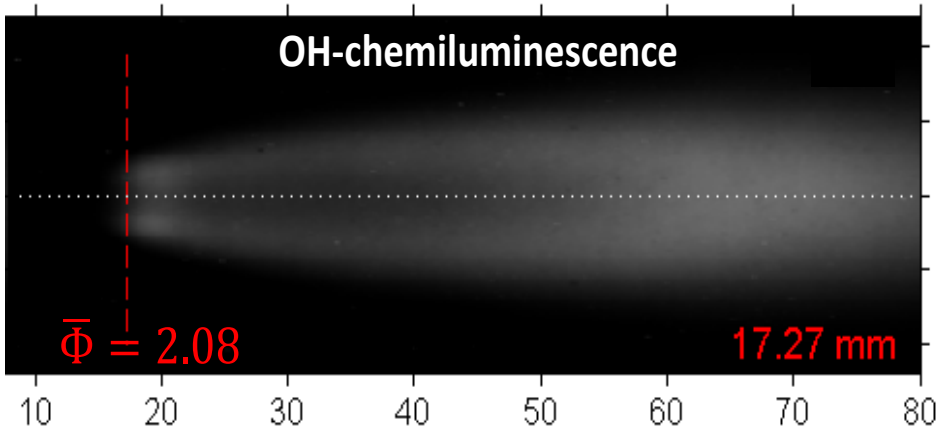
Spray-Combustion Simulation: Biodiesel

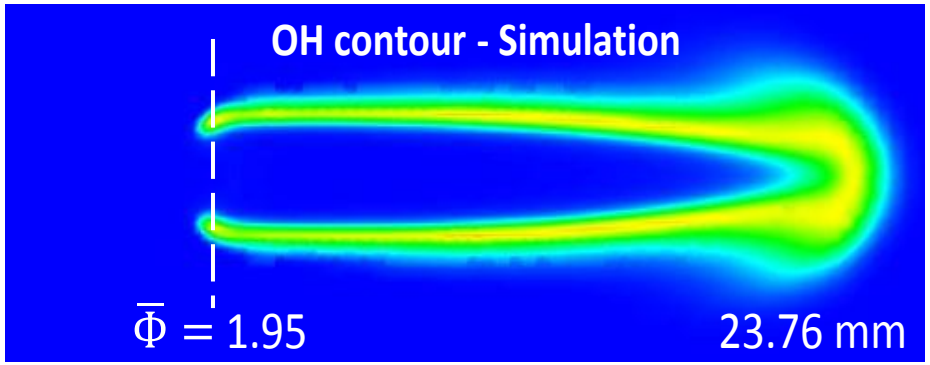
- ✓ 3D simulations: results on a cut-plane are animated
- ✓ Total of 550K-650K grid points for resolving a 108 mm (each side) cube
- ✓ 0.25 mm minimum grid size
- ✓ 4-5 days on 24 processors in the Fusion (Argonne) cluster



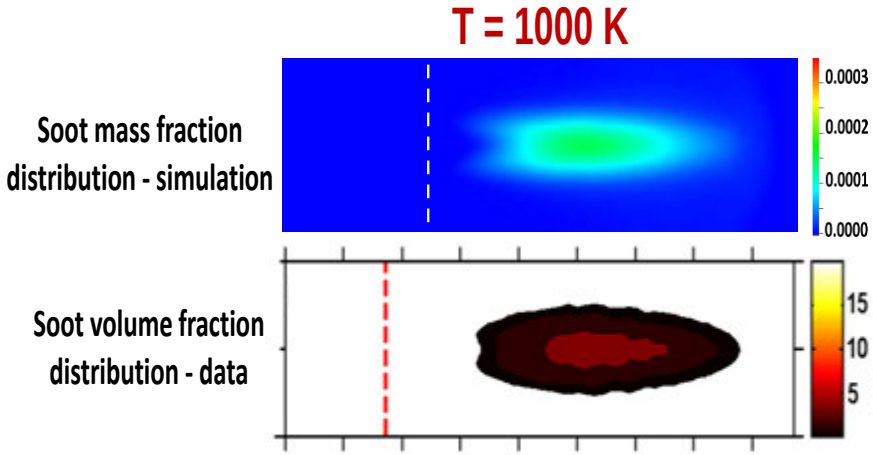
- ❑ Flame base moves back
- ❑ No flow structures
- ❑ Smooth profiles of temperatures

Validation: Turbulent Spray-Combustion Systems





Mixture Composition:
MB = 0.2, n-heptane = 0.8



- 25-30 % over-prediction of both ignition delay and flame lift-off lengths
- This is mainly due to the fact that MB+NHPT is still not a good surrogate for biodiesel since Cetane numbers are fairly different

* Experimental Data: Pickett & Co-workers (2011) *Personal Communication*

JG Nerva, CL Genzale, JMG Oliver, LM Pickett. Fundamental Spray and Combustion Measurements of Biodiesel under Diesel steady conditions. *Under preparation*

Combustion modeling of diesel surrogates: Validation with ECN data

Team members:

Douglas E. Longman: Argonne

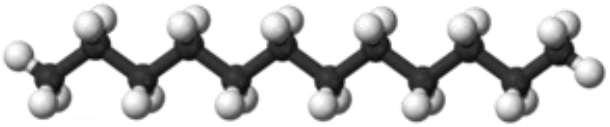
Mani Sarathy, Bill Pitz: Lawrence Livermore National Laboratory

Tianfeng Lu, Zhaoyu Luo: UConn

Lyle Pickett: Sandia National Laboratory

S. Som, Z. Luo, M. Plomer, W.J. Pitz, D.E. Longman, T. Lu. Development and validation of an n-dodecane skeletal mechanism for diesel spray-combustion applications. Submitted to *The Proceedings of the Combustion Institute*, 2012

Diesel surrogate:
n-dodecane ($nC_{12}H_{26}$)



Mechanism Reduction Methodology**

~ 20 times reduction

Detailed Mechanism (from LLNL)
2115 species, 8157 reactions

DRG – X*

369 species,1495 reactions

DRGASA

Skeletal Mechanism:
103 species,
370 reactions

Range of operation:
- ✓ Pressure: 1-100 atm
- ✓ Equivalence ratio: 0.5-2.0
- ✓ Initial temperature: 700 – 1800 K

* T. Lu, M. Plomer, Z. Luo, S.M. Sarathy, W.J. Pitz, S. Som, D.E. Longman, 1A03. *US National Combustion Institute meeting, 2011*

** S. Som, Z. Luo, M. Plomer, W.J. Pitz, D.E. Longman, T. Lu, Submitted to *The Proceedings of the Combustion Institute*, 2012

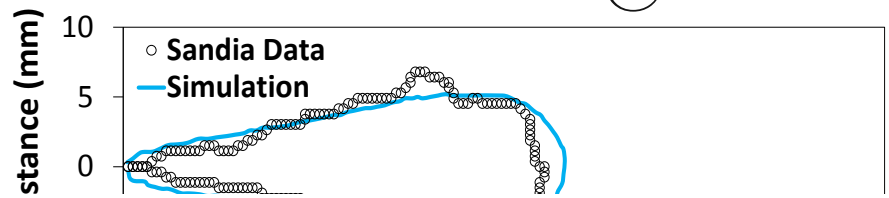
3D Spray (non-combust

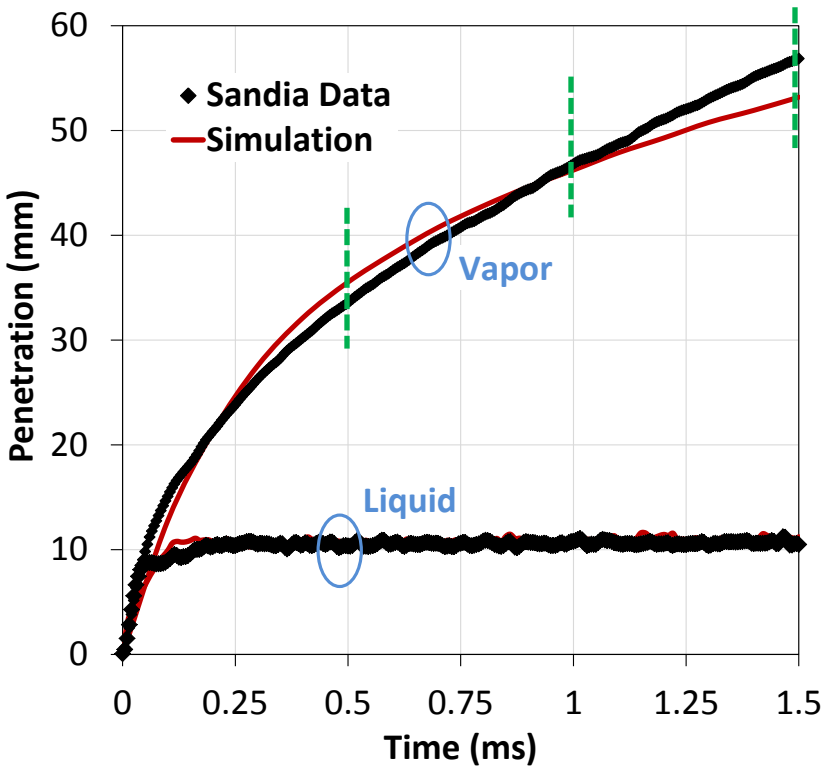
@ 900 K

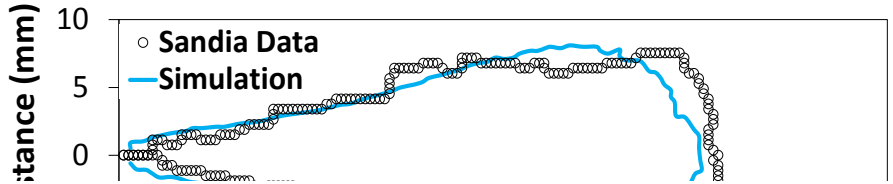
Data from Sandia National Laboratory:

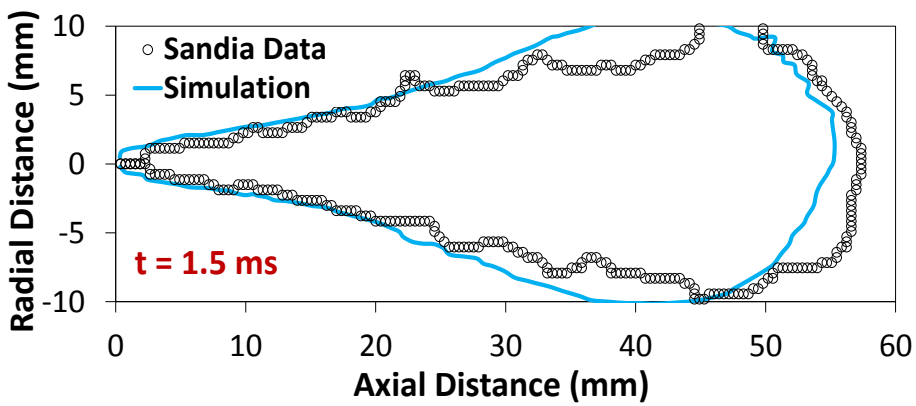
http://www.sandia.gov/ecn/

Simulation are able to capture the spray characteristics very well!





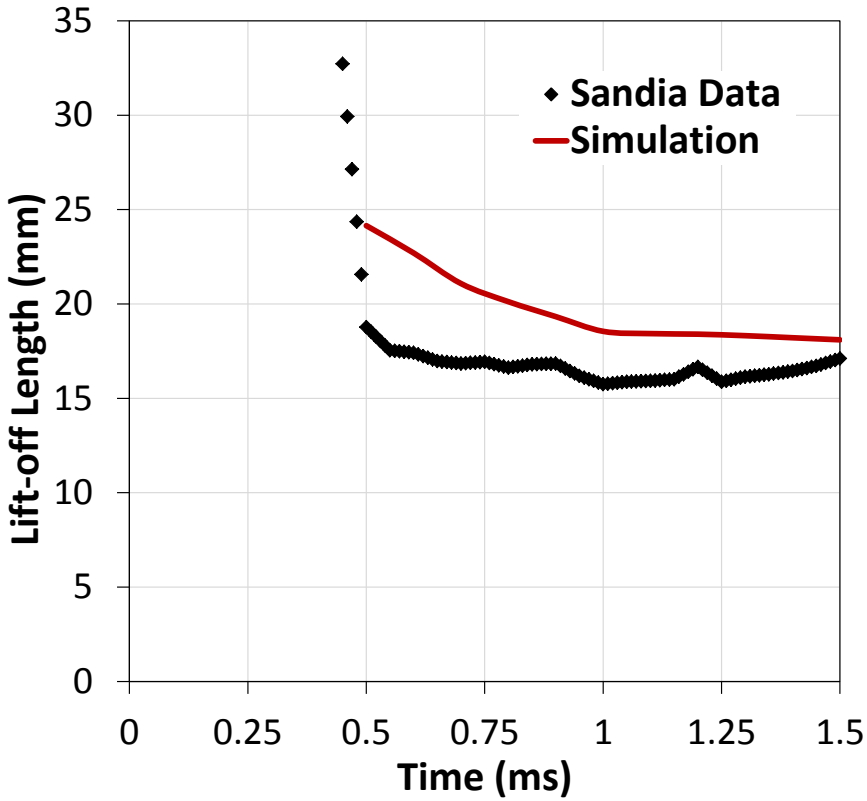




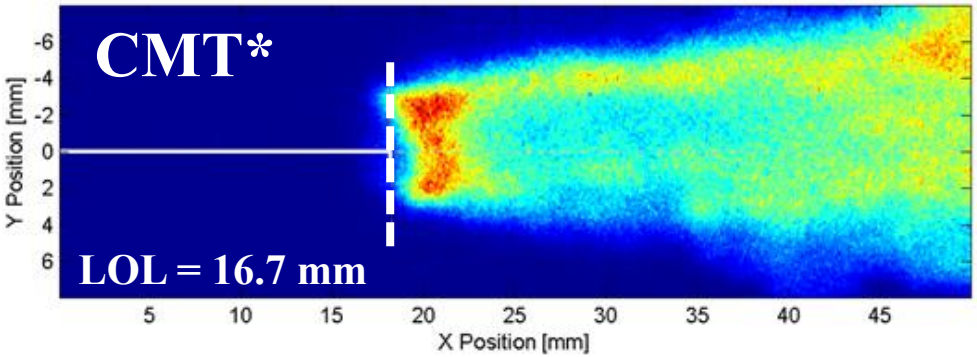
* S. Som, D.E. Longman, Z. Luo, M. Plomer, T. Lu. 26IC-0218. Fall technical meeting of the Eastern states of the combustion institute. October 2011.

Ignition Delay and Flame lift-off Length

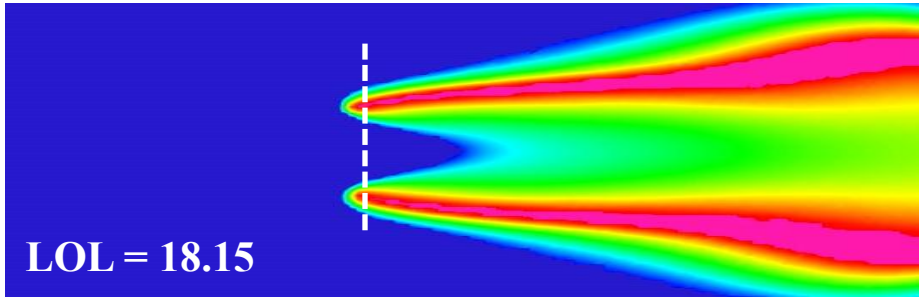
@ 900 K	Ignition Delay (ms)	Lift-off Length (mm)
Sandia Data	0.440	16.50
Simulation	0.455	18.15



OH chemiluminescence

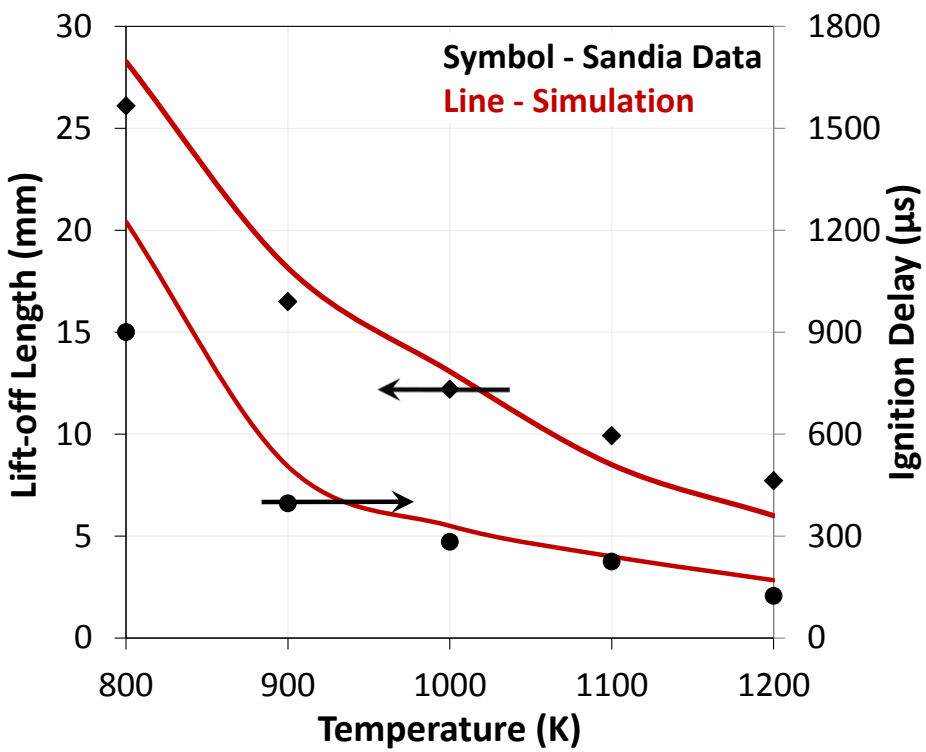


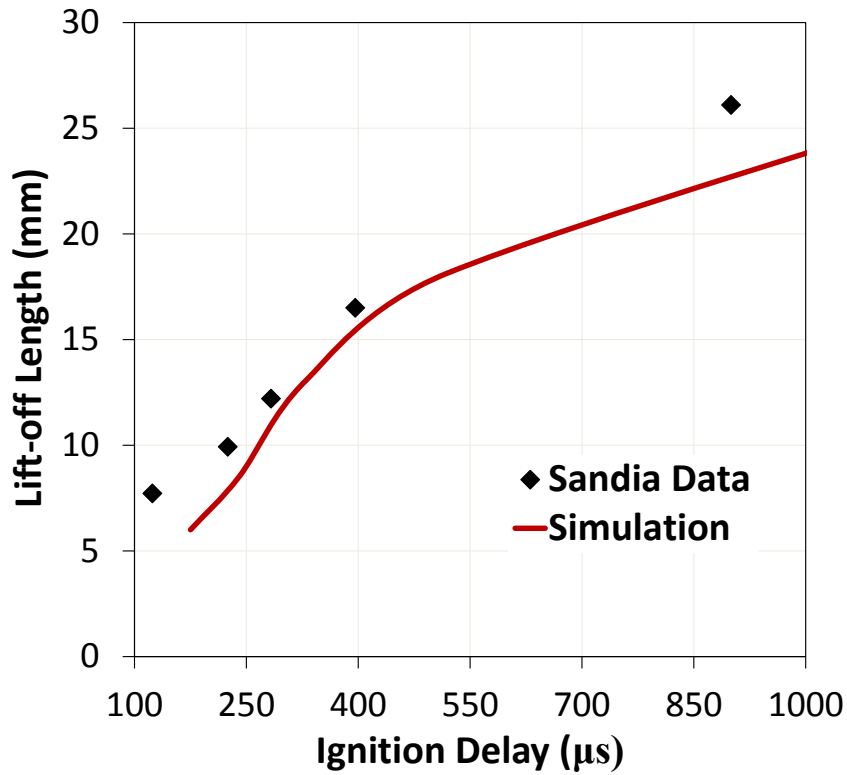
Simulation



*http://www.cmt.upv.es/ECN07.aspx

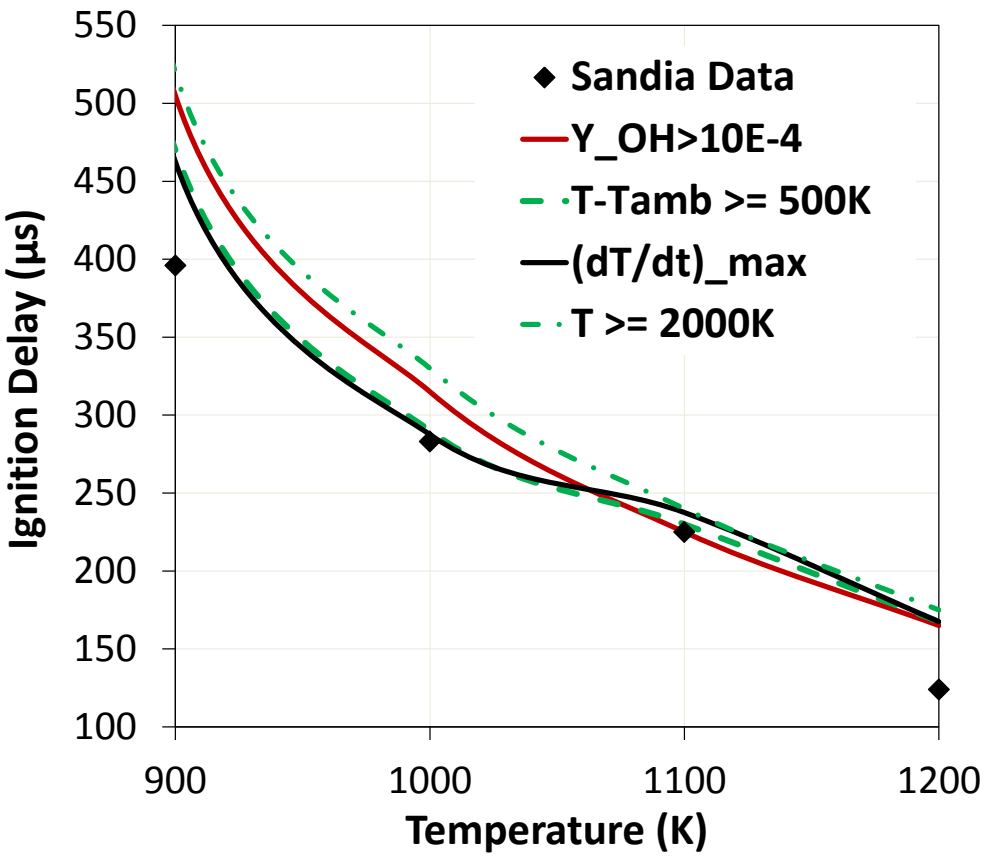
Effect of Ambient Temperature

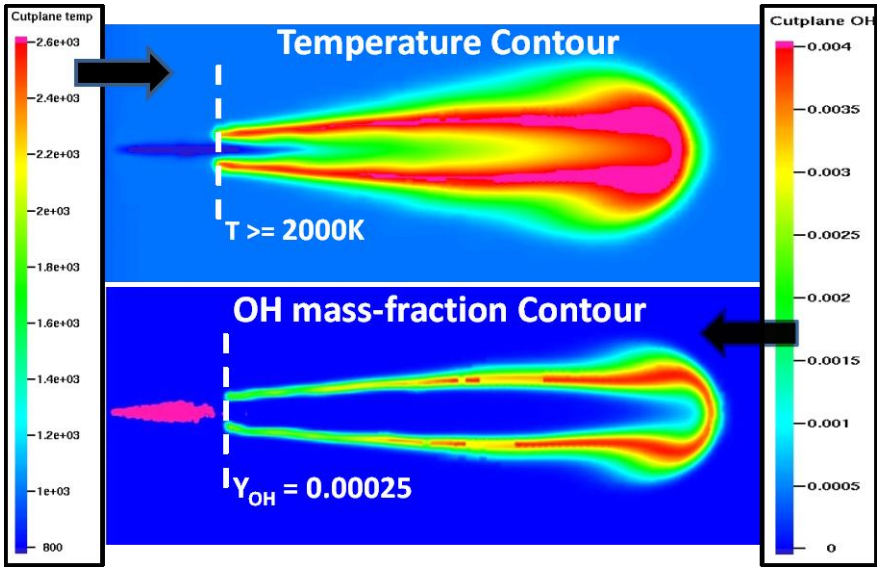




- At ambient temperatures of 900, 1000, and 1100 K the mechanism is able to capture the ignition delay and flame lift-off trends well
- Discrepancies are observed at low and high temperatures and we are working with LLNL and UConn to further resolve them
- Lower ignition delay results in lower lift-off lengths

Definition of Ignition and Flame Lift-off Length





Data: http://www.sandia.gov/ecn/

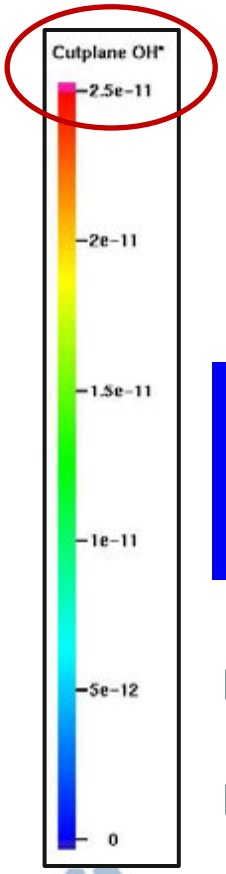
- Small differences are observed in predicted ignition delays and flame lift-off lengths based on definitions chosen
- 0-D simulations using CHEMKIN can show up to 10-20% difference in ignition delays based on definitions such as $(dT/dt)_{max}$, $(dY_{OH}/dt)_{max}$

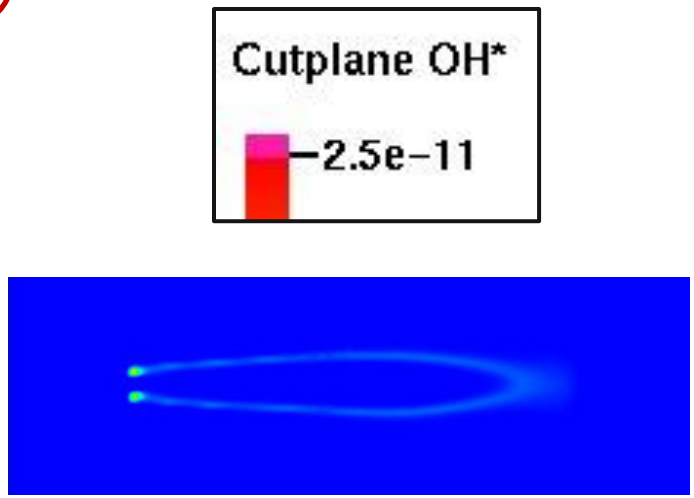
Is OH* an Accurate Indicator of Ignition?

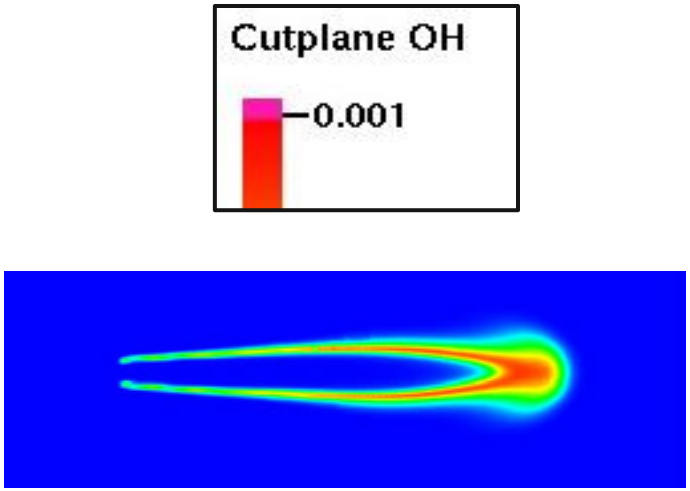
CH+O2=CO+OH*	4.800E+16	-1.0	5100	!Hall and Petersen, IJCK 06
H+O+M=OH*+M	3.800E+14	0.0	10000	!Hall and Petersen, IJCK 06

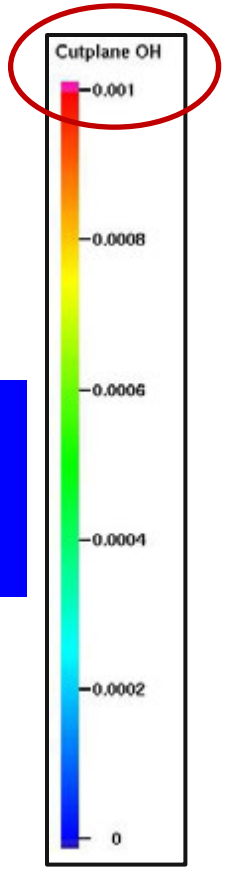
Total 15 reactions: Provided by Bill Pitz (Personal communication)

Flame structure at 2.0 ms









- OH* concentrations too low for using as a realistic indicator for ignition
- LLNL further investigating various other pathways which can lead to OH* formation

Large Eddy Simulation using Smagorinsky Model

Team members:

Eric Pomraning, Peter K. Senecal: Convergent Science, Inc.

S. Som, P.K. Senecal, E. Pomraning. Comparison of RANS and LES Turbulence models against constant volume diesel experiments. ILASS Americas 2012, San Antonio, USA

N-heptane mechanism: 68 species, 168 reactions (Lu et al.): Combustion and Flame 2009.

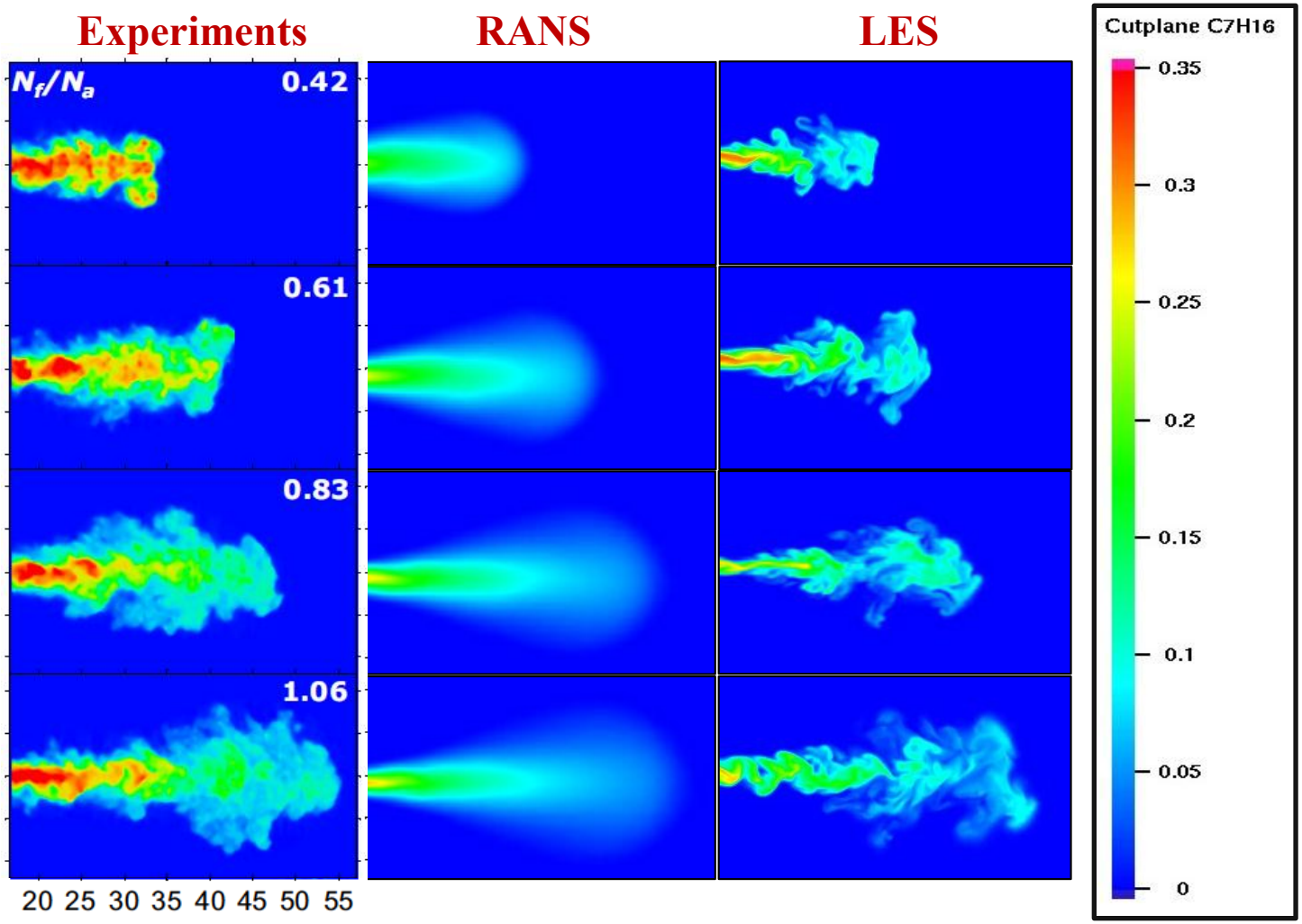
LES Modeling with Detailed Chemistry

Smagorinsky based LES Model:

- ✓ 0.125 mm minimum grid size
- ✓ Total of 2 millions grid points for resolving a 108 mm (each side) cube
- ✓ 8-10 days on 24 processors in the fusion cluster

Instantaneous Equivalence Ratio Distribution

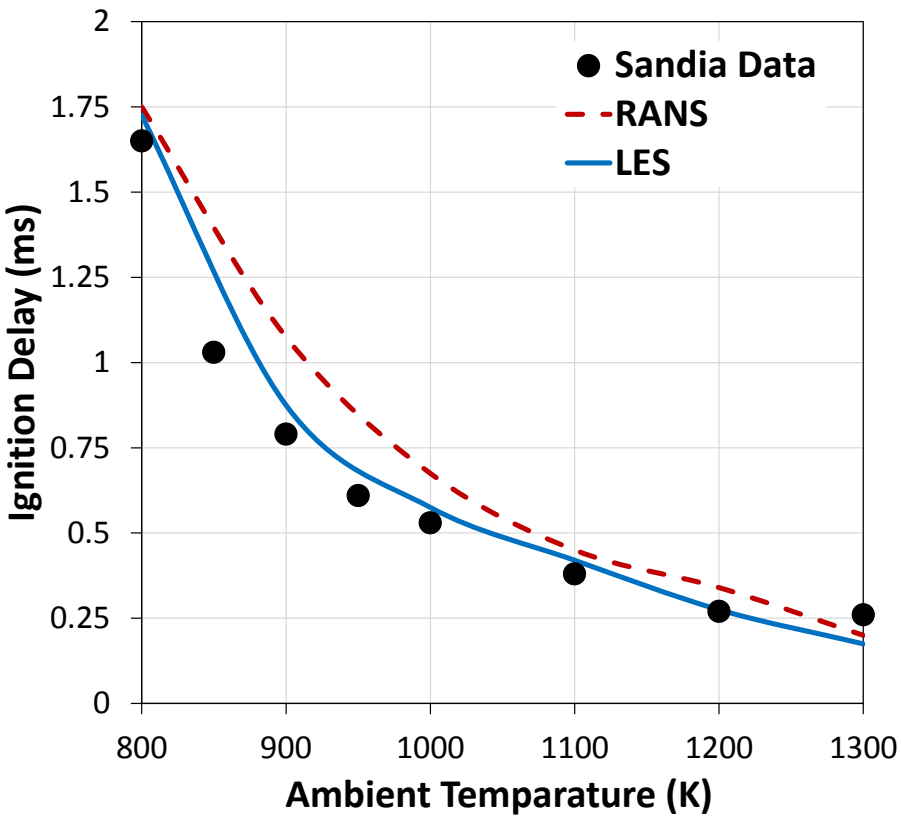
http://www.sandia.gov/ecn/

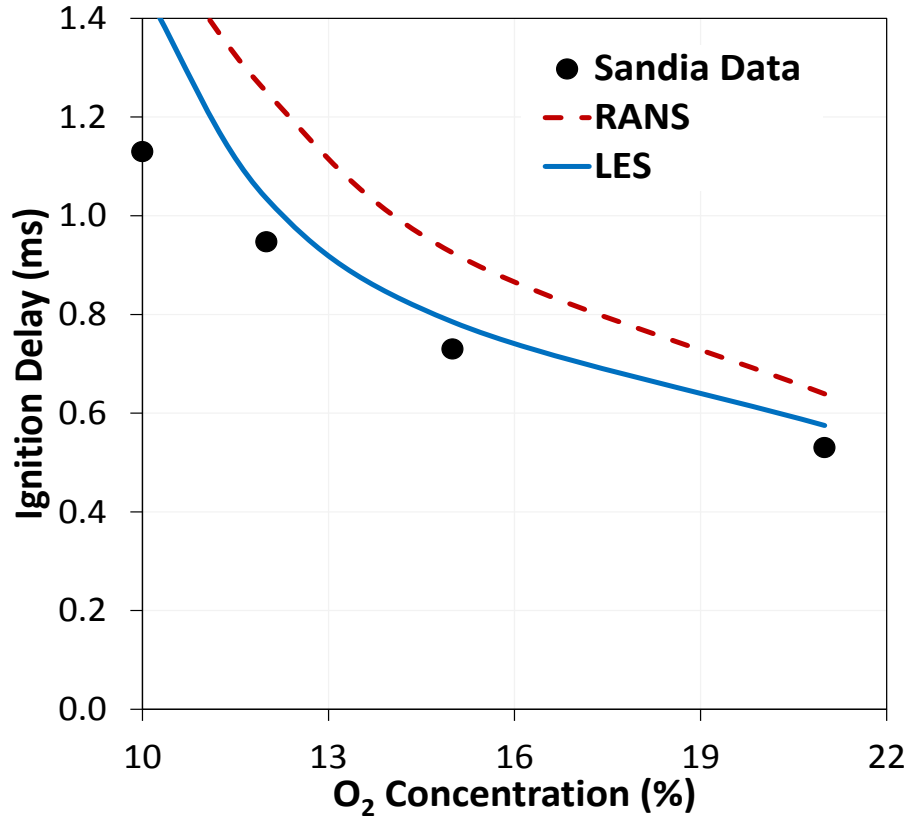


n-heptane: T_{amb}=1000K, ρ_{amb}=14.8Kg/m^3, O_2 Concentration = 0%,

Orifice diameter = 100µm, P_{inj}=1500bar, T_{fuel}=373K

RANS vs. LES: Ignition Delay*





- Earlier ignition with LES under all conditions investigated
- Quasi-steady Lift-off length values with RANS and LES are similar

* S. Som et al. Simulating flame lift-off characteristics of diesel and biodiesel fuels using detailed chemical kinetic mechanisms and LES turbulence models. ASME-ICEF2011-60051, October 2011, Morgantown, USA.

Nozzle flow simulations: Comparison of diesel with heavy-alcohol-diesel blends

Team members:

Anita Ramirez, Douglas E. Longman (Argonne)

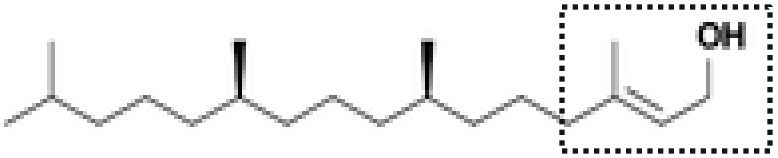
Phil Laible (Biophysicist): Argonne

Ramirez AI, Som S, LaRocco LA, Rutter T, Longman DE. Investigating the use of heavy alcohols as blending agent for compression ignition engine applications. ICES 2012-81169, *ASME-ICED Spring Technical Conference*, Italy, May 2012

Phytol-Diesel blends

- Metabolic engineering efforts at Argonne have designed strains that can be produced in large quantities by photosynthetic bacteria eventually producing a heavy alcohol called Phytol ($C_{20}H_{40}O$).

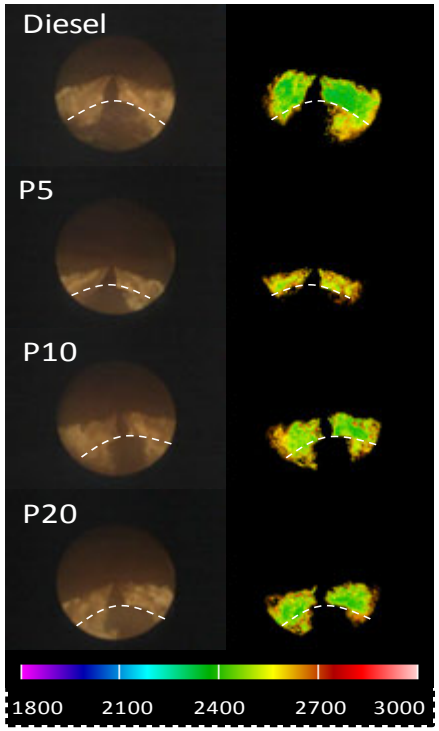
Phytol ($C_{20}H_{40}O$)
tetramethyl-2-hexadecen-1-ol

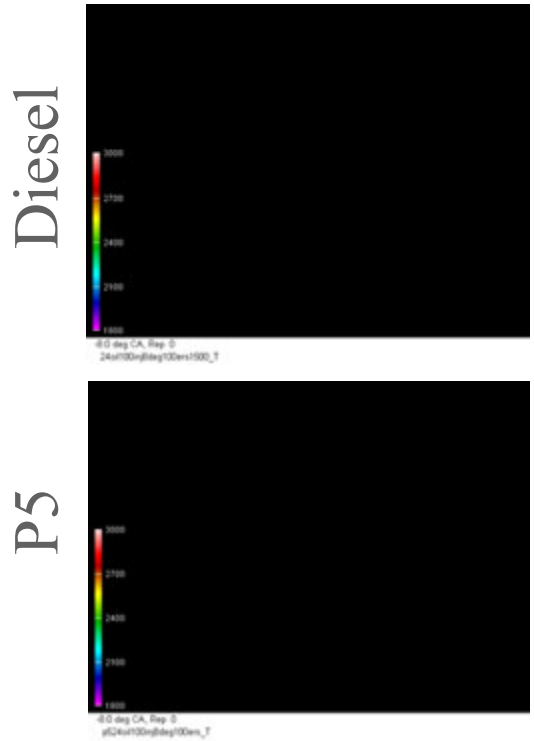


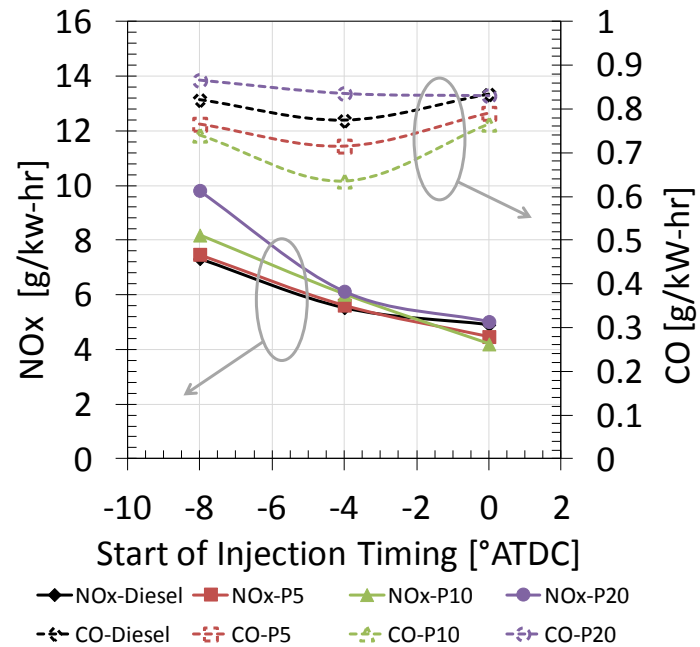
- The physical and chemical properties such as density, cetane number and heat of combustion are close to that of diesel fuel

Fuel Property	Diesel	Phytol	P-5	P-10	P-20
Carbon Content [wt %]	86.64	80.62	86.54	85.87	85.47
Hydrogen Content [wt %]	13.01	13.5	13.14	13.11	13.19
Sulphur content [ppm]	11.2	< 10	10.3	10.5	< 10
Heat of Combustion [KJ/Kg]	44,500	43,600	45,400	45,400	45,100
Cetane Number	47-48	45-46	47-48	46-47	45-46
Density @ 25˚C [Kg/m^3]	849.2	850.9	849	849	849.2
Vapor pressure @ 25˚C [Pa]	1000	< 1			
Viscosity @ 25˚C [cSt]	3.775	63.54	4.115	4.69	6.142

Engine Combustion Results

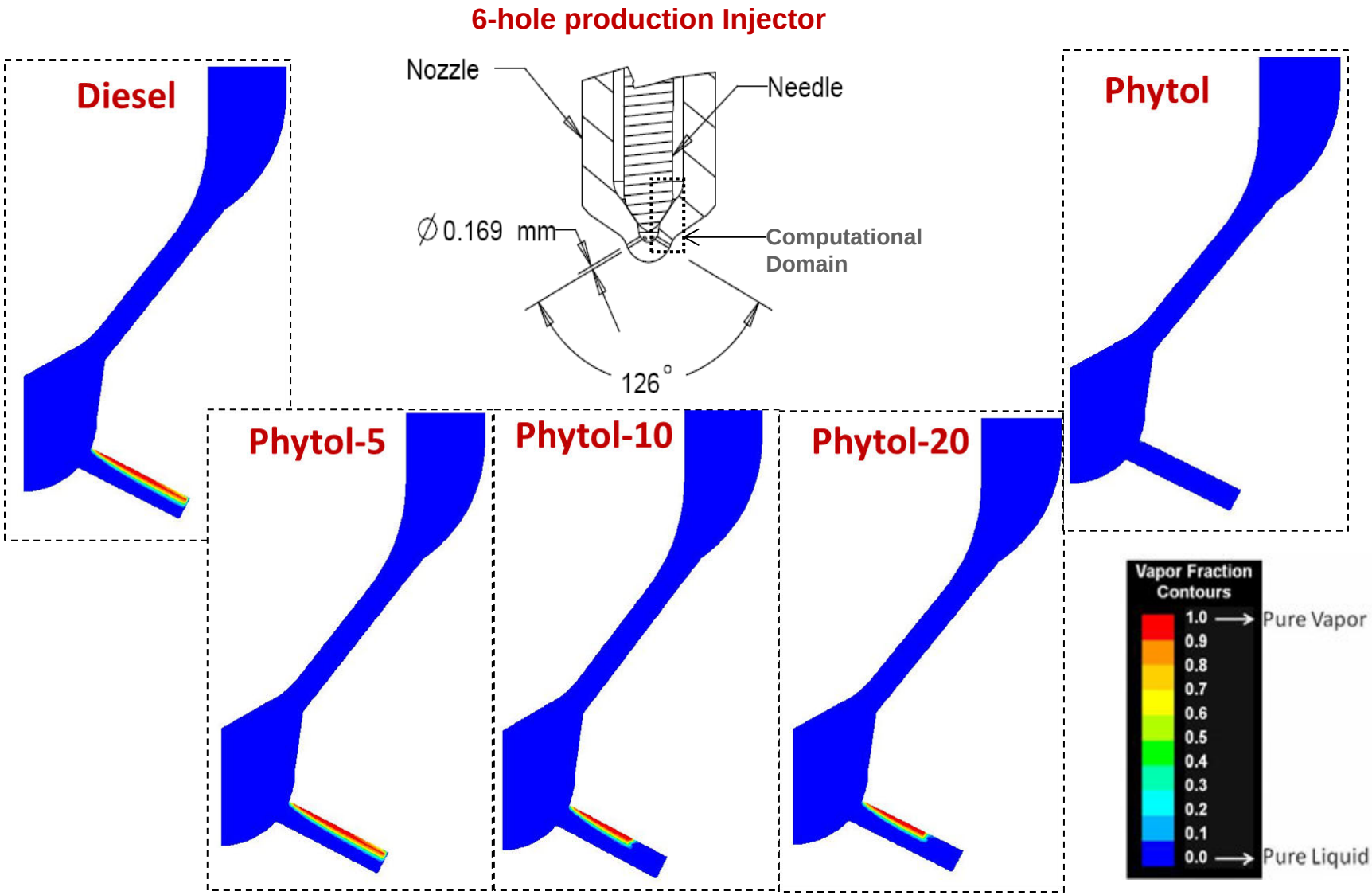






- Although the cylinder pressure traces showed little discernible differences, optical imaging showed higher temperatures for the P20.
- A slight reduction in CO emissions was seen when using the P5 and P10 blends while NO_x remained comparable.
- When there is 20% blending by volume, both experiments and simulations show that the physical and chemical properties may have been affected appreciably and influenced spray, combustion, and emission behavior.

Vapor Distribution



* Ramirez AI, Som S, LaRocco LA, Rutter T, Longman DE. ICES 2012-81169, *ASME-ICED Spring Technical Conference*, Italy, May 2012

Future Work

- Modeling: From shock-tubes to engines
  - ✓ Study the sensitivity of key reactions on ignition in 0D and 3D systems
  - ✓ Couple the fuel chemistry with a relevant NOx model
- Spray combustion modeling with diesel surrogates
  - ✓ Continue working with LLNL on improving the fidelity of n-dodecane mechanism for 3D simulations
  - ✓ Collaborate with LLNL on a n-dodecane + m-xylene mechanism, validation with ECN data
- Spray-combustion modeling with phytol-diesel blends
  - ✓ Collaboration with LLNL for heavy-alcohol mechanism
  - ✓ Spray modeling using KH-ACT primary breakup model

Thank You!

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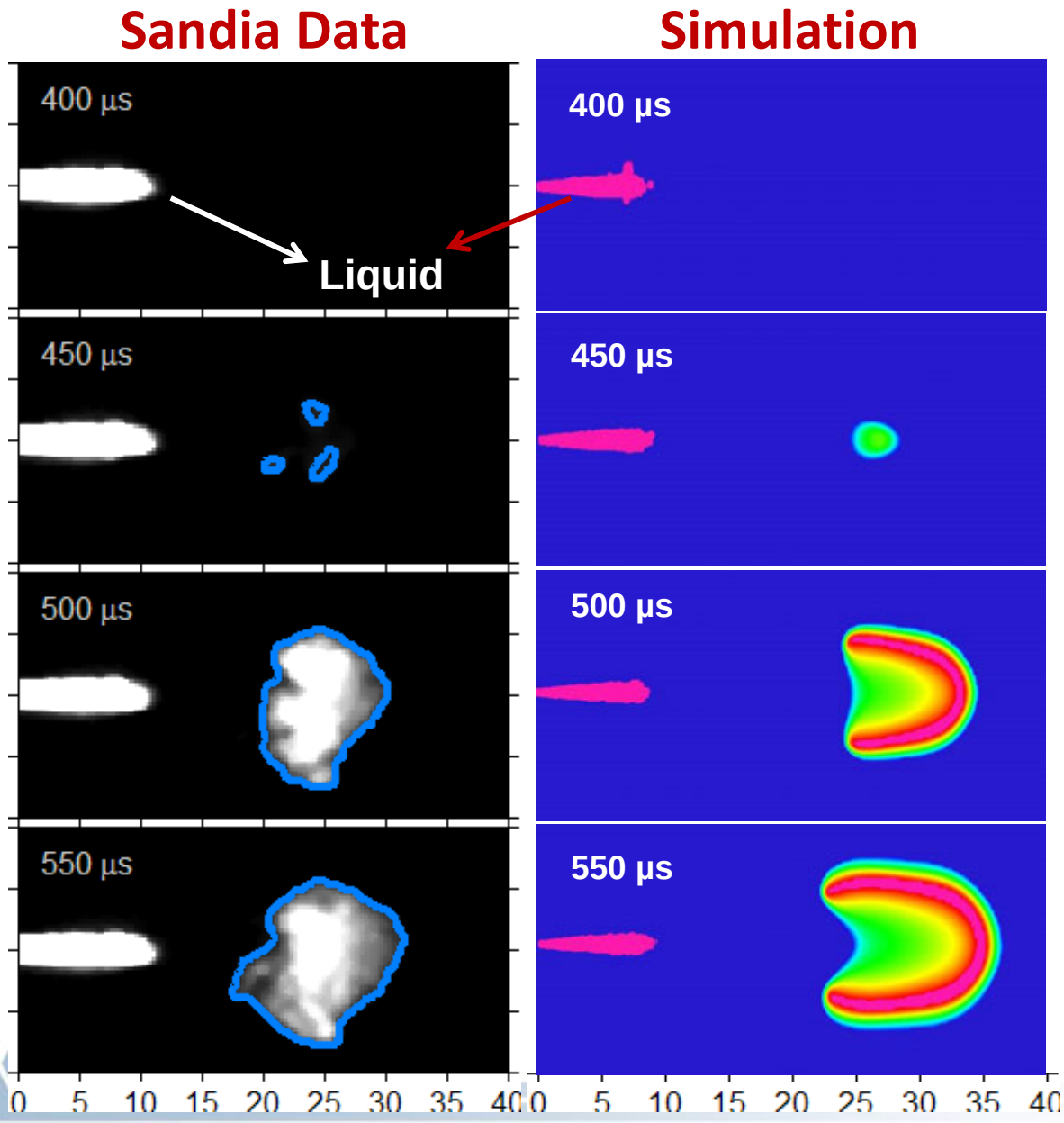
Contact: ssom@anl.gov

http://www.transportation.anl.gov/engines/multi_dim_model_home.html

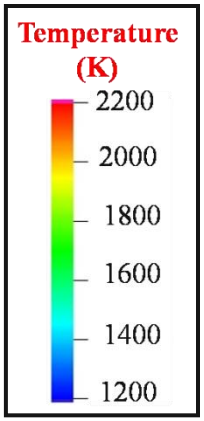
Liquid Length and Ignition Location



@ 900 K

Experiments:
Natural Luminosity high-speed imaging for detection of ignition delay
http://www.sandia.gov/ecn/

Simulation:
Temperature contours plotted to capture ignition location and delay



All OH* reactions

```
CH+O2=CO+OH*                    4.800E+16   -1.0    5100   !Hall and Petersen, IJCK 06
H+O+M=OH*+M                     3.800E+14    0.0   10000   !Hall and Petersen, IJCK 06
H+OH+OH=OH*+H2O                 1.450E+15    0.0     0.0   !Smith et al. 2005
!OH*+AR=OH+AR                   2.170E+10    0.5    2057
OH*+H2O=OH+H2O                  5.920E+12    0.5   -8.61E2
OH*+CO2=OH+CO2                  2.750E+12    0.5   -9.68E2
OH*+CO=OH+CO                    3.230E+12    0.5   -7.87E2
OH*+H=OH+H                      1.500E+12    0.5     0.0
OH*+H2=OH+H2                    2.950E+12    0.5   -4.44E2
OH*+O2=OH+O2                    2.100E+12    0.5   -4.82E2
OH*+O=OH+O                      1.500E+12    0.5     0.0
OH*+OH=OH+OH                    1.500E+12    0.5     0.0
OH*+CH4=OH+CH4                  3.360E+12    0.5   -6.35E2
!OH*=OH+HV                      1.400E+06    0.0     0.0
OH*+N2=OH+N2                    1.080E+11    0.5    -1238
```

LES Turbulence Model

The density weighted LES spatial filtering operation on the Navier-Stokes equation results in the filtered momentum equation:

$$\frac{\partial \overline{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} - \frac{\partial \overline{\rho} T_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \tilde{u}_i}{\partial x_j}\right) - \overline{F_i}$$

where the LES sub-grid scale tensor: $T_{ij} = \left(\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j\right)$

is modeled using a Smagorinsky based model: $T_{ij} = -2C_s\Delta^2\left|\overline{S}\right|\overline{S_{ij}} + \frac{1}{3}\delta_{ij}T_{kk}$

where $\left|\overline{S}\right| = \sqrt{2\overline{S_{ij}}\,\overline{S_{ij}}}$ $\quad \Delta = V_{cell}^{1/3}$ $\quad \overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right)$

Sub-grid turbulent kinetic energy:

$$k \cong C_{les}\frac{\Delta^2}{24}\frac{\partial \overline{u_i}}{\partial x_j}\frac{\partial \overline{u_i}}{\partial x_j}$$

$C_s = 0.2$ $\qquad$ **$C_{les} = 2.0$**